INTERMEDIATE STATE THEORY OF SCATTERING RESONANCES[†]

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I. INTRODUCTION

The relationship between the single particle resonance of shell model potential and resonances associated with particle hole states is extremely crucial to a consistent, indeed a correct, calculation of a nuclear reaction cross section. In fact, a considerable amount of insight into the correctness or the usefulness of a particular formulation of reaction theory can be gained from the way in which single particle resonances are handled, particularly when they occur near thresholds. A resonance associated with any non-zero value of angular momentum becomes increasingly narrow if the resonance energy is decreased. Not only does the resonance then become more difficult experimentally to distinguish from a "compound nuclear resonance", but appreciable configuration mixing with discrete shell model states may make this distinction less meaningful. The single particle resonance is parceled out among more complex levels (e.g. two-particles, one-hole states) in precisely the manner discussed by Lane, Thomas, and Wigner[1]. We shall learn from our analysis of a low-lying resonance that in this situation the "doorway state" is a single particle state, or one quasiparticle state.

The considerations of this paper are based on the shell model reaction theory outlined in earlier papers[2], and the results of a specific calculation will be presented for the $d_{3/2}$ resonance in the elastic scattering of neutrons on O^{16}. For the purpose of testing a reaction theory the situation which obtains in the nuclei with A = 15,16, and 17 is nearly

ideal and this paper is preliminary to a more extensive survey of the reactions involving these nuclei.

The $d_{3/2}$ resonance observed in $O^{16}(n,n)O^{16}$ occurs at 0.934 MeV with a width of only 90 keV. This width is approximately what one should expect for a d-wave resonance produced by the average Hartree field in this nucleus. A corresponding resonance also occurs in proton scattering on O^{16}. Since these resonances arise from the average potential generated by O^{16}, we should also expect to find $d_{3/2}$ resonances in the nucleon scattering on O^{15} and N^{15}. In the simplest shell model these nuclei are described as belonging to the configuration $1p_{1/2}^{-1}$, a hole in the $1p_{1/2}$ shell. Overlooking the distinction between bound and continuum states for the moment, we could describe the resonance observed in nucleon scattering on N^{15} and O^{15} as "belonging to the configuration $p_{1/2}^{-1} d_{3/2}$". Similarly if elastic scattering could be performed on O^{15} and N^{15} in their first excited state ($p_{3/2}^{-1}$ in the shell model), resonances would be observed which could be described as "belonging to $1p_{3/2}^{-1} d_{3/2}$".

Now actually a central potential can only describe nucleon scattering in the lowest approximation, and therefore even the continuum states $p_{1/2}^{-1} d_{3/2}$ and $p_{3/2}^{-1} d_{3/2}$ are not eigenstates of the complete Hamiltonian with a real two-body interaction. A diagonalization of the full Hamiltonian using just these continuum states will yield eigenstates which are a linear superposition of these two configurations. Such a calculation is

equivalent to finding the inelastic scattering which is produced by the two-body interaction by a direct interaction.

The calculation of the nucleon scattering is further complicated, however, by the fact that discrete bound states belonging to the configurations $p_{1/2}^{-1} d_{5/2}$, $p_{3/2}^{-1} d_{5/2}$, $p_{1/2}^{-1} 2s_{1/2}$, and $p_{3/2}^{-1} 2s_{1/2}$ also interact strongly with the resonant continuum states (which have large amplitudes over the nuclear volume). In the shell model calculations of the bound and the "resonant states" of O^{16} a $d_{3/2}$ state is included among the particle states from which the particle-hole states are constructed. Since a bound $d_{3/2}$ state does not actually exist in O^{17}, it is clear that such a state is actually a representative of the $d_{3/2}$ single particle resonance. The conventional shell model diagonalization can then be viewed in some sense as an approximate diagonalization of the full Hamiltonian on the discrete shell model states and on certain <u>resonant</u> continuum states[3].

This description of the role of resonant continuum states is accurate, but it does not readily lend itself to an accurate calculation of the detailed shape of resonances, particularly when two or more resonances overlap. Therefore we shall develop another formulation which does provide a basis for such analyses. The motivation for the development of the next section is provided by the observation that a slightly deeper $d_{3/2}$ potential would provide a bound $d_{3/2}$ state. This state would then give discrete states of the configurations $p_{1/2}^{-1} d_{3/2}$ and $p_{3/2}^{-1} d_{3/2}$. The interaction of these states

would then easily be found by diagonalizing the Hamiltonian on this discrete set. We shall now proceed to show how to remedy the failure of nature to present us with this simpler situation.

II. RESONANCE THEORY OF SINGLE PARTICLE SCATTERING

We apply the formalism of the shell model reaction theory[2] to the analysis of low energy single particle resonance. Let U be a central potential which describes the elastic scattering and which therefore fits the resonance. For the purpose of the subsequent analysis we regard the cross section given by U as exact. The T- matrix element is

$$T(\vec{k}',\vec{k}) = \left\langle \Phi_{\vec{k}'} \mid U \mid \chi_{\vec{k}}^{+} \right\rangle \tag{1}$$

where $\Phi_{\vec{k}'}$ is a plane wave of mementum $\vec{k}'$ and $\chi_{\vec{k}}^{+}$ is the exact scattering wave function for the potential U with outgoing scattered waves at infinity.

Introduce now the potential $\hat{U}$ which is sufficiently deeper than U to possess a bound single particle state of the same quantum numbers as the sharp resonance of U. The energy of this state will be denoted by $E_d (= - E_B$, the binding energy). Let $\hat{H} = K + \hat{U}$ be the "model Hamiltonian", and use the scattering states $\hat{\chi}_k^{+}$ of $\hat{H}$ to calculate $T(\vec{k}', \vec{k})$.

Using the equation

$$\chi_{\vec{k}}^{+} = \hat{\chi}_{\vec{k}}^{+} + (E^{+} - \hat{H})^{-1} \Delta \chi_{\vec{k}}^{+} \tag{2}$$

where

$$\Delta \equiv U - \hat{U},$$

we can obtain by operator algebra[4]

$$T(\vec{k}', \vec{k}) = \left\langle \Phi_{\vec{k}'} \right| \hat{U} \left| \hat{\chi}_{\vec{k}}^{+} \right\rangle + \left\langle \hat{\chi}_{\vec{k}'}^{-} \right| \mathscr{T} \left| \hat{\chi}_{k}^{+} \right\rangle. \quad (3)$$

The "reduced transition operator" $\mathscr{T}$ is given by the equation

$$\mathscr{T} = \Delta + \Delta (E^{+} - \hat{H})^{-1} \mathscr{T}. \quad (4)$$

This equation is the starting point for our development of a resonance theory of single particle scattering.

Since the potential $\hat{U}$ will not have a resonance at low energy, $\mathscr{T}$ is the quantity which introduces a resonance into the scattering amplitude. This resonance can be exhibited explicitly by separating $\mathscr{T}$ into a non-resonant "effective interaction" $\hat{\mathscr{T}}$ and a resonant term of the Breit-Wigner form. The $\hat{\mathscr{T}}$ is defined by the equation

$$\hat{\mathscr{T}} = \Delta + \Delta (E^{+} - \hat{H})^{-1} P_{c} \hat{\mathscr{T}} \quad (5)$$

where P_{c} projects on the continuum states of H. From Eqs. (4) and (5) it follows that

$$\mathscr{T} = \hat{\mathscr{T}} + \hat{\mathscr{T}} P_{d} (E^{+} - \hat{H} - P_{d} \hat{\mathscr{T}} P_{d})^{-1} P_{d} \hat{\mathscr{T}}, \quad (6)$$

where P_{d} projects on the discrete bound state of $\hat{H}$ which corresponds to the narrow resonance of H. The T-matrix amplitude is then given by

$$T(\vec{k}', \vec{k}) = \left\langle \Phi_{\vec{k}'} \right| \hat{U} \left| \hat{\chi}_{k}^{+} \right\rangle + \left\langle \hat{\chi}_{\vec{k}'}^{-} \right| \hat{\mathscr{T}} \left| \hat{\chi}_{\vec{k}}^{+} \right\rangle$$
$$+ \frac{\left\langle \hat{\chi}_{\vec{k}'}^{-} \right| \hat{\mathscr{T}} \left| d \right\rangle \left\langle d \right| \hat{\mathscr{T}} \left| \hat{\chi}_{\vec{k}}^{+} \right\rangle}{E - E_{d} - S + i \frac{\Gamma_{d}}{2}} \quad (7)$$

The denominator of the resonance term is defined by

$$S - i\Gamma_{d/2} = \left\langle d \middle| \hat{\mathscr{T}} \middle| d \right\rangle \tag{8}$$

with S being called the level shift and Γ_d being the level width of the state. Both S and Γ_d are dependent upon the energy of the incident nucleon, but at resonance $E_d + S(E_R) = E_R$, the resonance energy, and $\Gamma_d(E_R)$ is the width of the single particle resonance.

The effective interaction, which determines the resonance energy and width through Eq. (9), is itself non-resonant. In a lowest approximation $\hat{\mathscr{T}}$ is just equal to Δ, the perturbation which pushes the bound state of H into the continuum and mixes it with the continuum levels of H. The deviation of $\hat{\mathscr{T}}$ from Δ arises from virtual transitions into continuum states with a consequent modification of the perturbing interaction. The optical theorem for $\hat{\mathscr{T}}$

$$\mathrm{Im}\,\hat{\mathscr{T}} = -\pi\,\hat{\mathscr{T}}\,P_c\,\delta\,(E^+ - \hat{H})P_c\,\hat{\mathscr{T}}^\dagger \tag{9}$$

leads to the familiar expression for Γ_d

$$\Gamma_d(E) = 2\pi\,\left| \left\langle d \middle| \hat{\mathscr{T}} \middle| \hat{\chi}^+(E) \right\rangle \right|^2 \rho(E) \tag{10}$$

As should be anticipated from this view of matters, there is a simple relation between S and Γ_d. This is easily found by writing the explicit equation for $\hat{\mathscr{T}}$

$$\hat{\mathscr{T}} = \Delta + \Delta\,P_c\,(E^+ - P_c\,H\,P_c)^{-1}\,P_c\,\Delta \quad . \tag{11}$$

Find the states $\psi^+(E)$ which diagonalize $P_c\,H\,P_c$, i.e.

$$\left\langle \psi^{+}(E') | P_c H P_c | \psi^{+}(E) \right\rangle = E \, \delta(E-E') \qquad (12)$$

and use these to deduce from Eq. (8)

$$\Gamma_d(E) = 2\pi \left| \left\langle d \mid \Delta | \psi^{+}(E) \right\rangle \right|^2 \rho(E) \qquad (13)$$

$$S(E) = \left\langle d | \Delta | d \right\rangle + (2\pi)^{-1} \mathcal{P} \int dE' \, \frac{\Gamma_d(E')}{E - E'} \qquad (14)$$

The second of these two equations leads to an extremely simple way of calculating the energy dependent level shift to second order in Δ.

III. NUMERICAL EXAMPLE

This approach was used to describe the $d_{3/2}$ resonance at 0.934 MeV in elastic neutron scattering O^{16}. For simplicity U was chosen to be a square well whose depth and radius were chosen to fit the resonance energy and the width at half maximum respectively. The well $\hat{U}$ was also chosen as a square well, and with the same radius as U. The depth of $\hat{U}$, however, was chosen to give a bound state whose energy was varied from $E_d = 0$ to $E_d = -10$ MeV as a check on the sensitivity of the calculation to the choice of E_d. The results were found to be very insensitive to this quantity and we quote only the results for the calculation with $E_d = -0.1$ MeV.

After determining U and $\hat{U}$, we first calculated the resonance energy $E_R = E_d + S$ and $\Gamma(E_R)$ in the lowest approximation for $\hat{\mathcal{J}} = \Delta$. The resonance energy $E_R^{(1)}$ was found to be $E_R = 1.009$ MeV and width at resonance was approximately 100 keV. Since $\Gamma_d^{(1)}(E)$ is a function of energy from which the

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second order correction to the level shift is calculated, its
dependence on E was calculated for the range $0 \leq E \leq 50$ MeV and
is shown in Fig. (2).

The energy shift was then calculated to second order
using the equation

$$S^{(2)} = \langle d|\Delta|d \rangle + (2\pi)^{-1} \mathcal{P}\!\!\int dE' \frac{\Gamma_d^{(1)}(E')}{E-E'} \qquad (15)$$

Since the second order correction given by the last term of
this equation is a function of energy, we plot it in Fig. (3).
Notice that it is very small and is smoothly varying through
the resonance region around 1 MeV. The dependence of $S^{(2)}$
on the energy, however, means that the resonance energy $E_R^{(2)}$
must be found by solving the equation

$$E_R^{(2)} - E_d - S(E_R^{(2)}) = 0. \qquad (16)$$

The resonance energy is found to be $E_R^{(2)} = 0.937$ MeV. Within
the accuracy of our calculation this is the exact resonance
energy.

The width is much more difficult to calculate to second
order in Δ. Therefore we adopted another method of estimating
the effect upon Γ_d of the second order correction to $\tilde{\mathcal{F}}$. Make
the approximation

$$\tilde{\mathcal{F}} = \theta \Delta \qquad (17)$$

where θ is a constant whose magnitude is fixed by the exact
resonance energy.

$$E_R = 0.934 \text{ MeV} = E_d + \theta \langle d | \Delta | d \rangle \qquad (18)$$

The width is then calculated with this approximation to and is found to be 90 keV at resonance.

The scattering cross section is proportional to $\sin^2 \delta_{3/2}$. As a further check on the intermediate state representation of the resonance cross section, the quantity $\sin^2 \delta_{3/2}$ was calculated from Eq. (7) using $E_d + S = 0.934$ MeV and $\Gamma_d(E) = 2\pi |\langle d | \theta \Delta | \hat{\chi}^+ \rangle |^2 \rho(E)$ for all energies. The result agreed with the exact calculation of $\sin^2 \delta_{3/2}$ to better than 1% except where the cross section was small or rapidly varying. Maximum errors of 3% at such places are obviously a consequence of the crude approximations used in evaluating the resonance amplitude.

IV. SUMMARY

The significance of our work is that we have shown that narrow, single-particle resonances are easily treated by introducing a bound state which plays the role of an intermediate state in a Breit-Wigner resonance amplitude. The resonance energy and the width of the state are determined by a one-body effective interaction which is non-resonant. This means that the $d_{3/2}$ resonance observed in nucleon scattering on O^{16} can be incorporated into the shell model by introducing a $d_{3/2}$ bound state, which is then treated on the same footing as the other bound single-particle states. In O^{16} this $d_{3/2}$ state can be combined with the $1p_{3/2}^{-1}$ hole states in the same way as

are the $1d_{5/2}$ and $2s_{1/2}$ bound states. The shell model diagonalization which is to be carried out with a particle-hole interaction will then include in a relatively simple way the effect of configuration interaction between all the resonant continuum states (associated with the $d_{3/2}$ single-particle resonance) and the bound states.

The only essential modification required of the particle-hole treatment of O^{16} is the addition of the one-body interaction in the $1d_{3/2}$ state. In the shell model diagonalization which leads to the resonant energies and the compound states the only effect of this additional interaction is to "restore" the $d_{3/2}$ single particle energy to the position of the resonance observed in O^{17}. The shell model calculation is then of same form as that of Elliot and Flowers,[5] G. E. Brown[6] and others.[7]

In the calculation of particle widths for the states of O^{16} the one-body interaction in the $d_{3/2}$ state is a direct consequence of the fact that this state is not bound. Consequently, even in the absence of a particle-hole interaction the 24.3 MeV state of O^{16}, which belongs mostly to $p_{3/2}^{-1} d_{3/2}$, would decay. This contribution to the particle width of the compound states is properly included by the procedure of this paper.

Finally, we wish to point out that the $d_{3/2}$ intermediate state introduced to describe the scattering resonance in O^{17} is properly regarded as a "doorway state" although this violates the common conception of such states. Such states are commonly

thought of as being states which differ from the initial state
by the excitation of a nucleon. In current parlance--"doorway
states" differ by two-quasi particles from the initial state.
More properly, however, a doorway state should be regarded as
merely a resonant configuration which is directly coupled to
the incident channel and also to more complex excitations of
the compound system. The $d_{3/2}$ state clearly meets this criterion.

The application of this formalism to a complete analysis
of the states of O^{16} is being carried out and will be reported
in another paper.

References

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Figure Captions

Figure 1.   The potential U provides the resonant $d_{3/2}$
scattering cross section which is regarded
as exact.   The potential $\hat{U}$ possesses the
bound $d_{3/2}$ state whose displacement by the
perturbation $\Delta = U-\hat{U}$ gives rise to the scat-
tering resonance of U.

Figure 2.   The width function $\Gamma_d^{(1)}$ calculated with
$\hat{\mathcal{T}} = \Delta$.

Figure 3.   The second order correction to the energy
of the intermediate state [c.f.Eq. (14)]
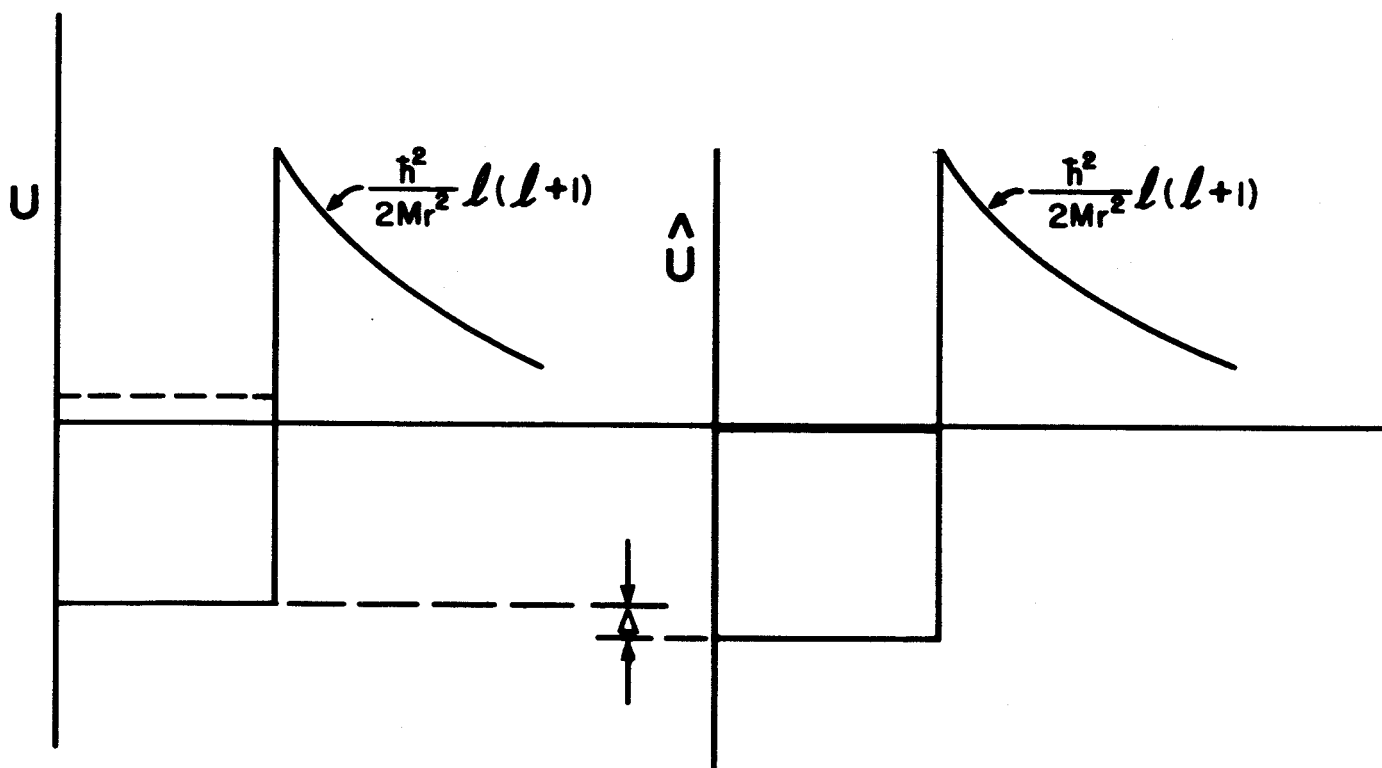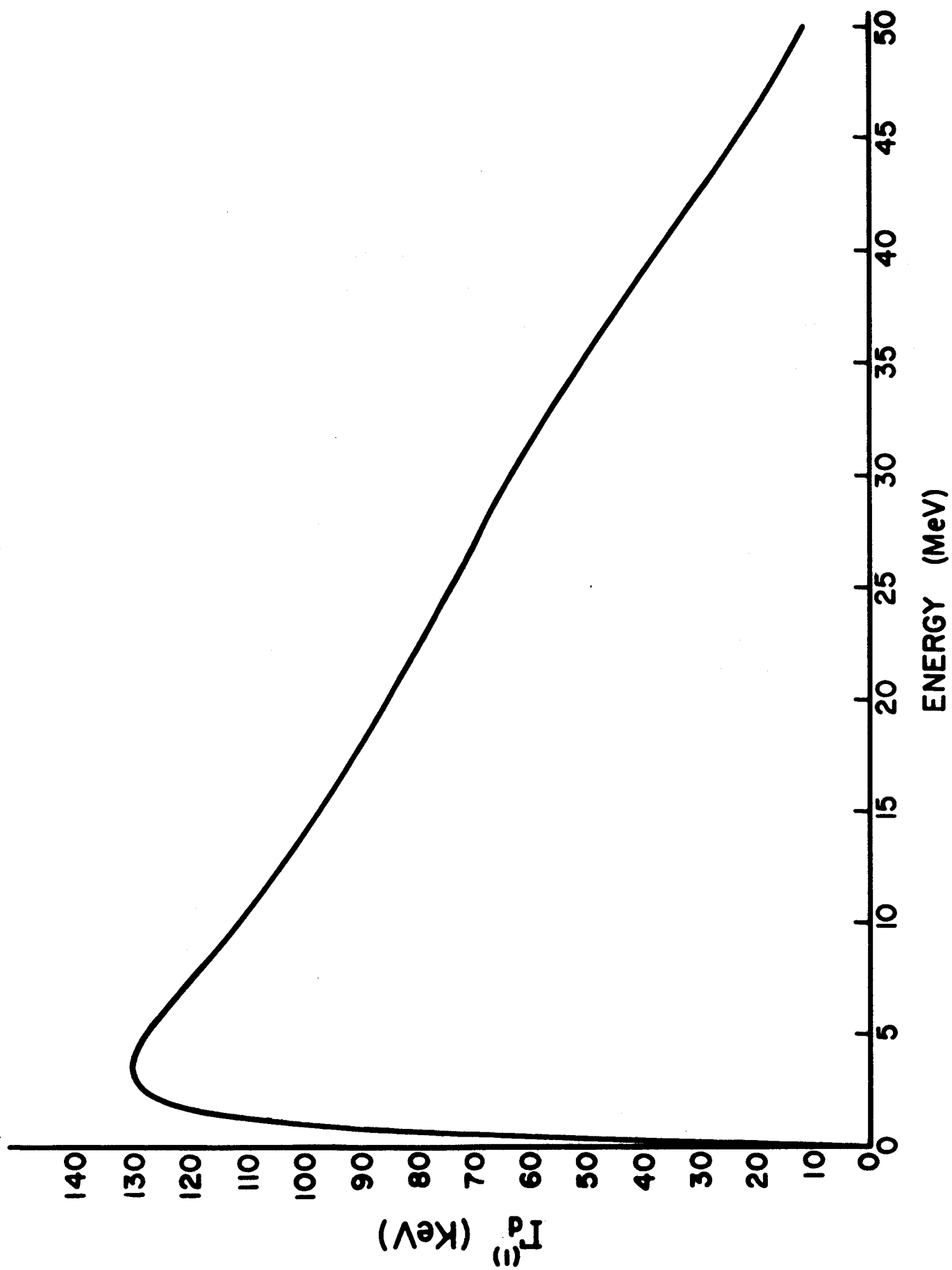is given as a function of the energy of the
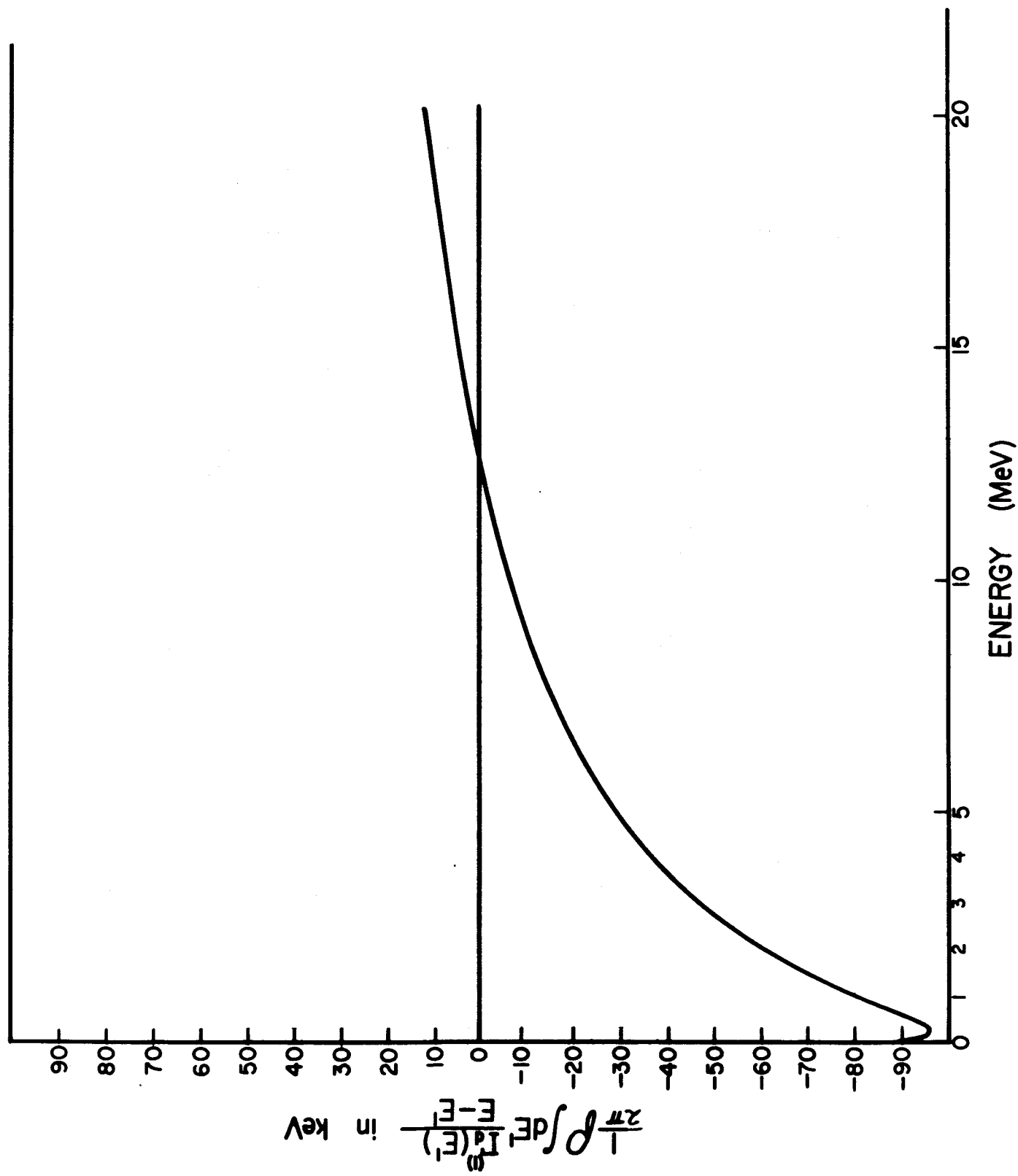incident nucleon.

Figure 1

Figure 2

ENERGY (MeV)

$$\frac{1}{2\pi}\mathscr{P}\!\int dE'\,\frac{\Gamma_0(E')}{E-E'}\quad\text{in keV}$$

Figure 3